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Associating GB Characteristics with its Sink Efficiency in Absorbing Frank Loops in Cu

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07/06/2021



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Motivation

- To investigate the interaction of the migrating GB with prismatic loops in Cu. More specifically, whether GBs get pinned by the loops, traverse the loops or absorb it, and how this interaction relates to the misorientation angle (low-angle vs. high-angle GBs) as well as the local GB structure.
- To this end, we have selected a set of low-angle and high-angle GBs for this study. The range of misorientation angle is $0^\circ \sim 60^\circ$. For some misorientation angles, multiple phases are studied to investigate the effects of local GB structure.

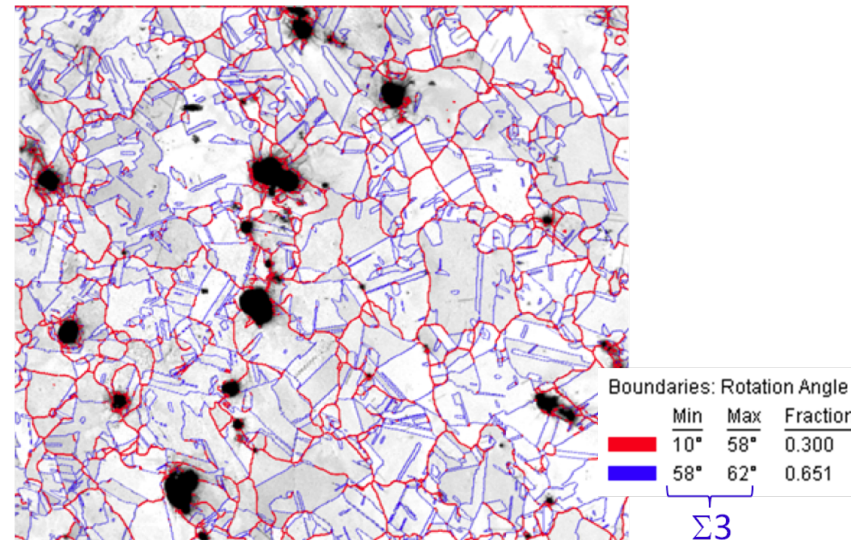
Relevant publications:

Associating GB characteristics with its sink efficiency in absorbing Frank loops in Cu, J Chen, K Dang, HT Vo, P Hosemann, SJ Fensin, Scripta Materialia 192, 61-66, 2021

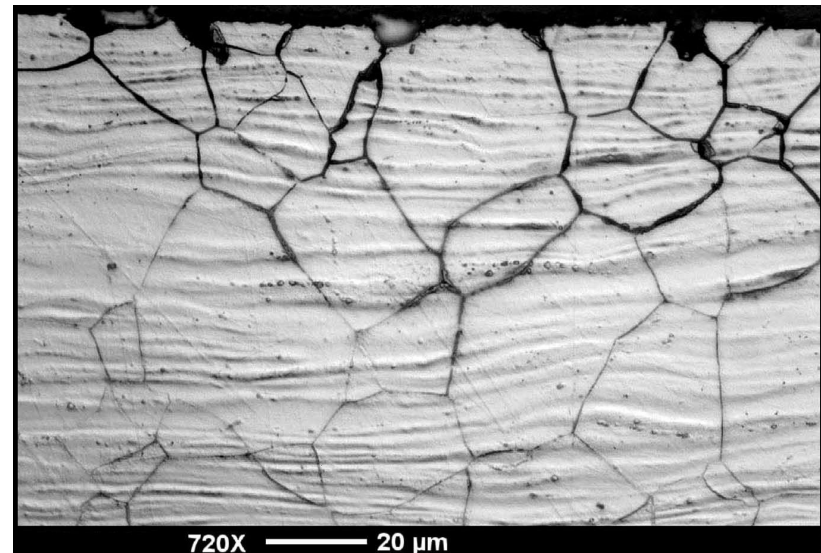
Why Do We Care about Grain Boundaries?

- Grain boundaries (GB) are internal interfaces formed when two misoriented crystal surfaces are brought together.
- GBs are the weak link for damage and failure under various types of loading conditions – active area of research.
- GBs can sometimes enhance corrosion in material by acting as transport channels for ions – active area of research.
- Due to the fine spatial and temporal resolution required to understand the role of grain boundaries in material behavior, atomistic simulations have been used.
- For tailored design of materials, it is important to understand and be able to predict material properties – GBs are a key to that

Dynamic Fracture

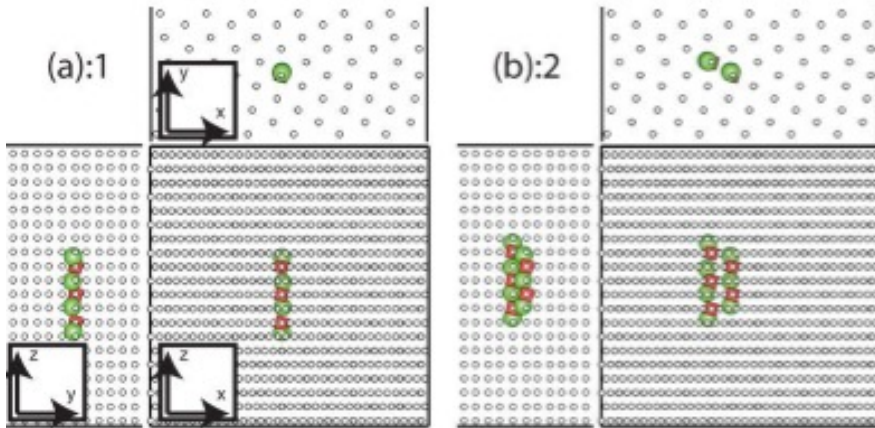


Intergranular Corrosion



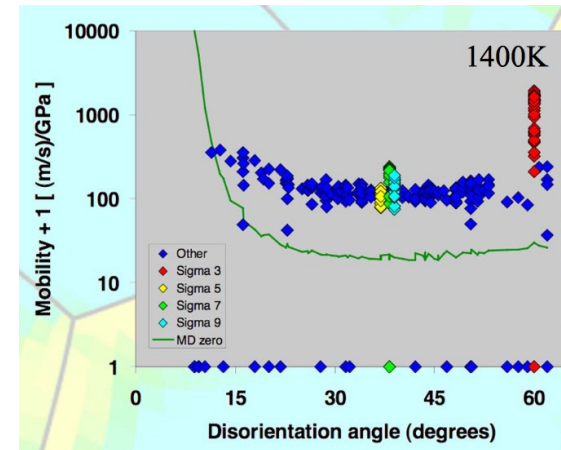
Atomistic Simulations Used to Understand Role of GBs in a Variety of Problems

Role of GB structure on defect structure and mobility



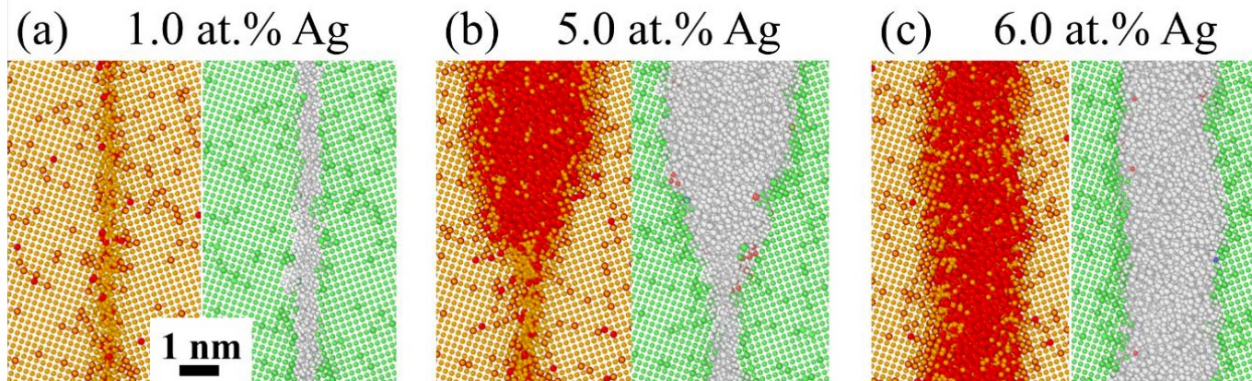
Uberuaga et al., 2015

Role of GB structure on mobility



Holm et al., 2012

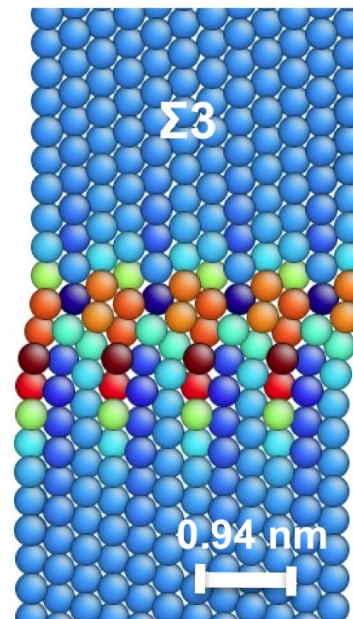
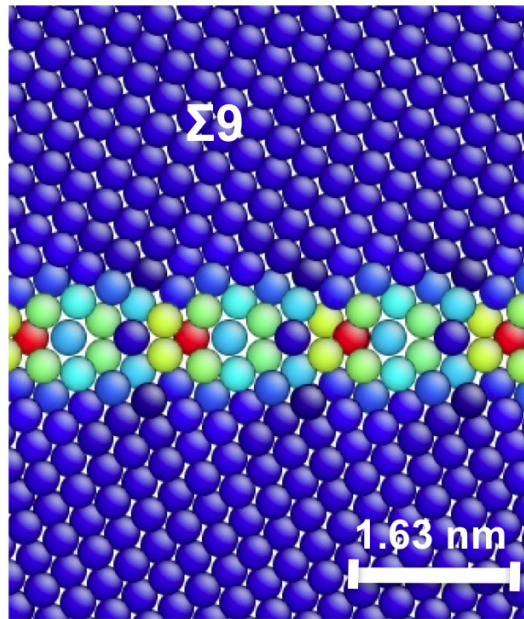
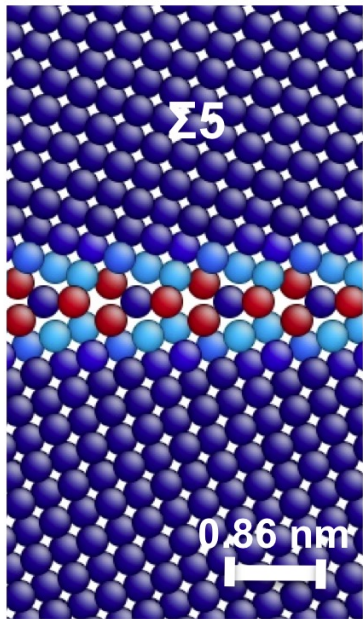
Role of GB structure on segregation



Rupert et al., 2018

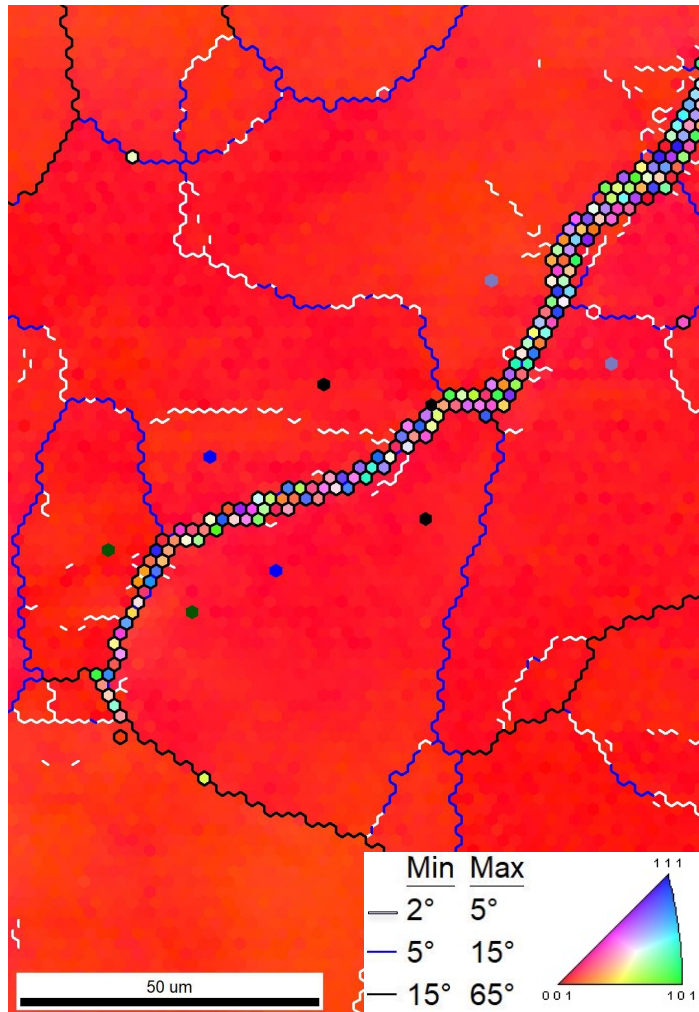
What Does Grain Boundary Structure Mean?

- In general terms, it is the arrangement of atoms at an interface
- In MD speak, the structure variation means changing the boundary type from a $\Sigma 3$ to 5 to 9... etc.
- We are usually limited by the constraints of the simulations – periodic boundary conditions, to only model special “ordered” boundary structured as defined by the coincident site lattice



- In these grain boundaries we are altering many parameters like misorientation not just the structure

Boundary Misorientation and Characteristic Changes along a GB



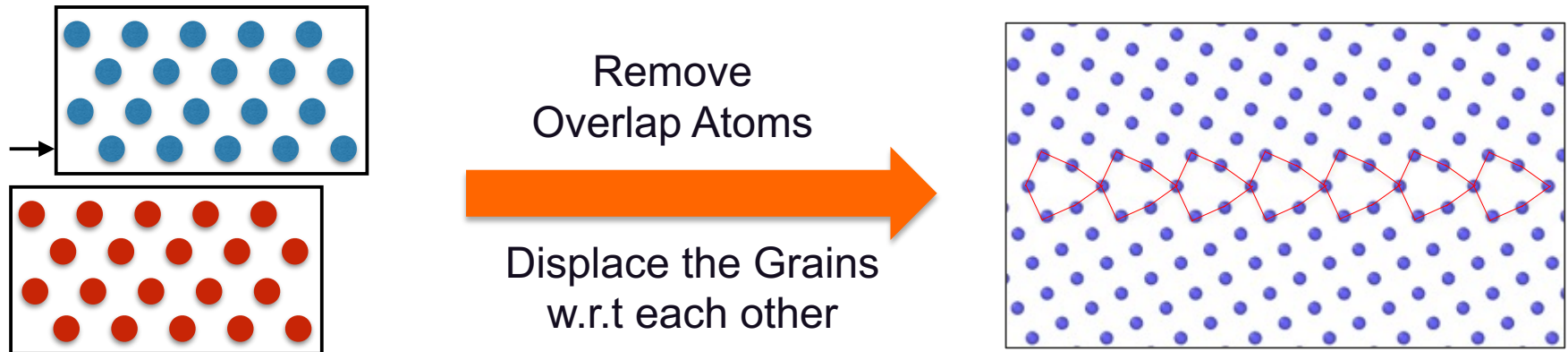
- Colored dot pairs are used to identify boundary misorientation and type along a boundary
- Misorientation across the boundary, as well as boundary type, varies along its length
- The grain boundaries are highlighted as follows: low angle boundaries are white (2°-5°) and blue (5°-15°), and high angle boundaries are black (15°-65°).

Color	Misorientation(p1)	Misorientation(p2)	Sigma	Deviation	Plane(p1)	Plane(p2)
●	39.67@[-1 1 30]	39.67@[-1 1 30]	5	2.98	[-18 1 0]	[18 -13 1]
●	31.43@[0 0 1]	31.43@[0 0 1]	5	5.46	[-22 7 1]	[1 -23 6]
●	33.88@[0 0 -1]	33.88@[0 0 -1]	5	3.02	[-6 26 -1]	[-10 -25 1]
●	24.13@[-2 20 -1]	24.13@[-2 20 -1]	13a	2.75	[-1 0 19]	[-8 -20 1]

Table 1: Misorientation and boundary type information

Real GBs are nothing like what is modeled in MD? So how do we get around that?

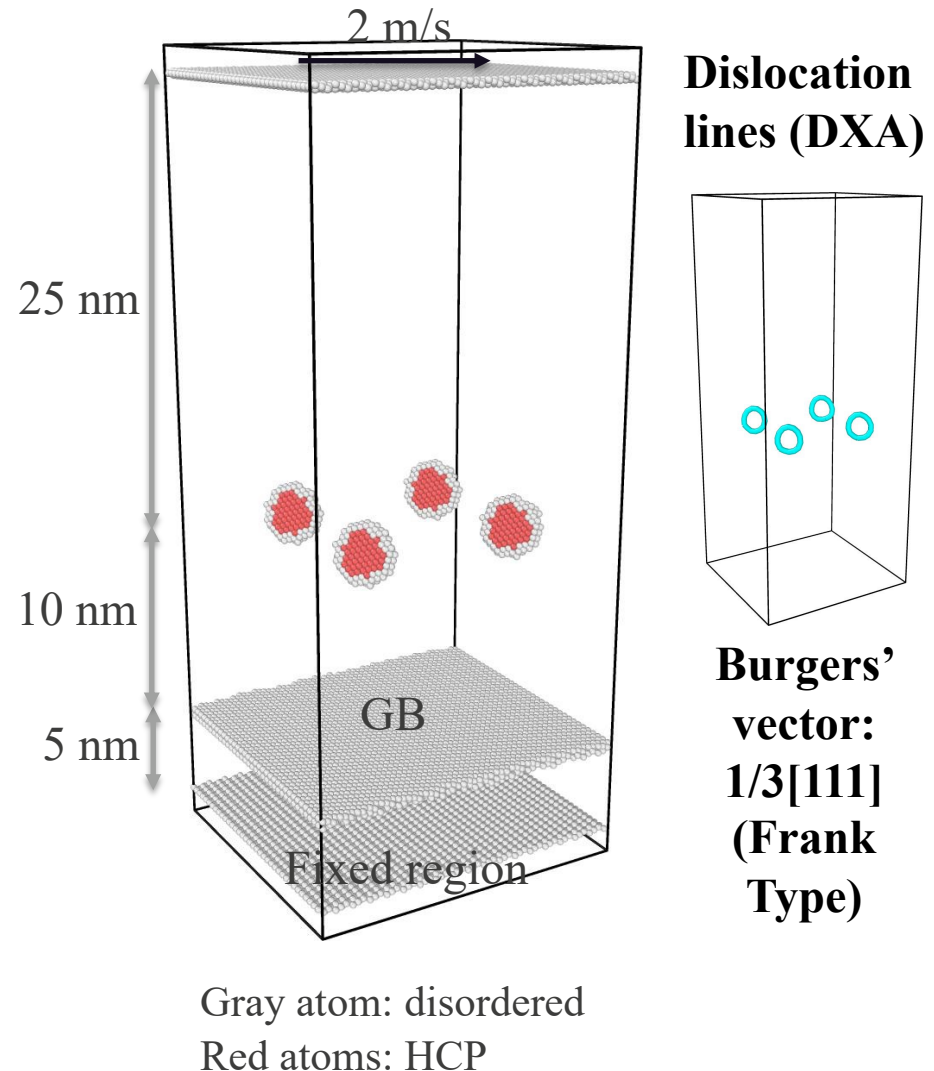
We propose to take Advantage of the the Common Methodology To Construct GB Structures



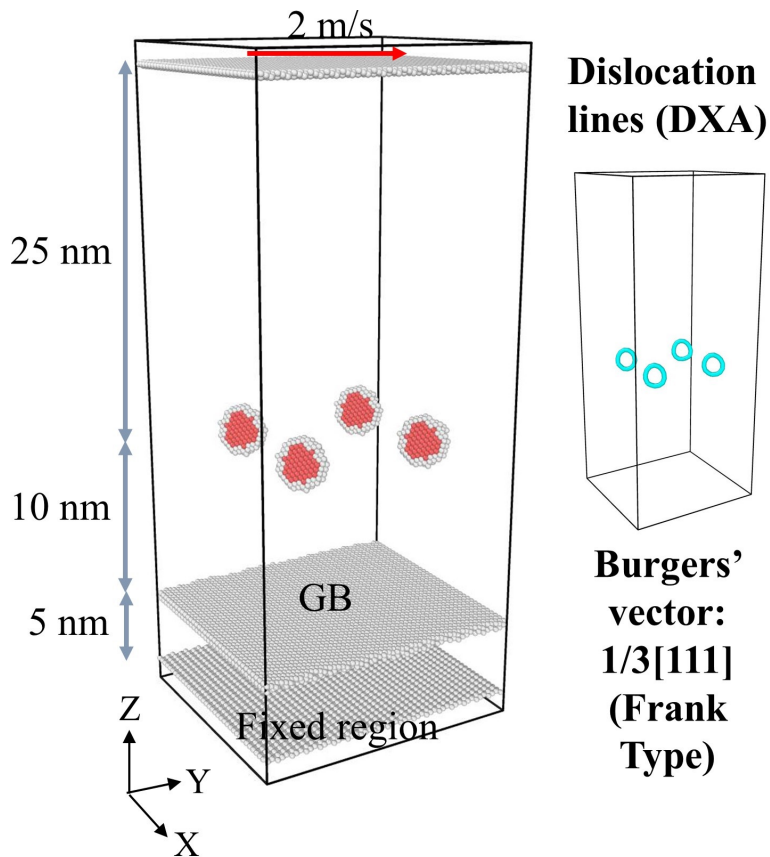
- This technique results in the formation of 100's of GB structures
- **Most researchers only choose the “minimum” grain boundary structure and use to to assess properties – hence the popularity of $\Sigma 3$ type boundaries.**
- **We argue that this is the wrong thing to do**
- A “real” grain boundary is probably a combination of all these structures
- We propose to calculate properties (energy, mobility, spall strength) for all these boundaries and then perform some form of averaging.

MD: Shear simulation setup

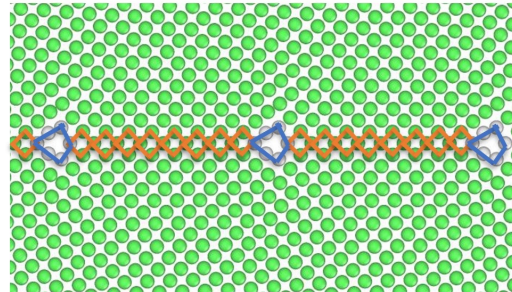
- System: Cu, 15 x 15 x 35 nm, ~ 500k atoms, with 4 circular prismatic loops (interstitial type, $D = 2$ nm) placed at 10 nm above a planar GB.
- Method: constant velocity shear of 2 m/s applied to the top control region, while the bottom control region is held fixed. Shear strain rate $\sim 5.7 \times 10^8 \text{ s}^{-1}$.
- Temperature: 10 K.
- Potential: EAM potential by Mishin et. al.



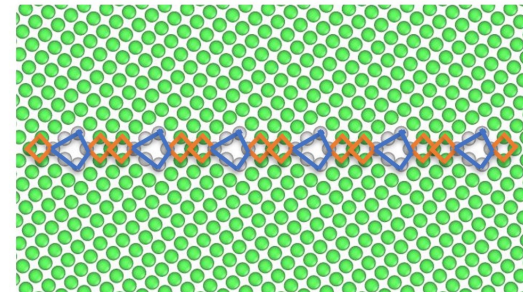
GB Structure Altered such that the number of Structural Units A and B would Vary



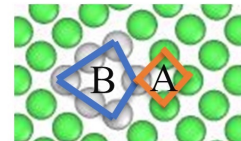
$\Sigma 181(0\ 9\ 10): |8A-B|$



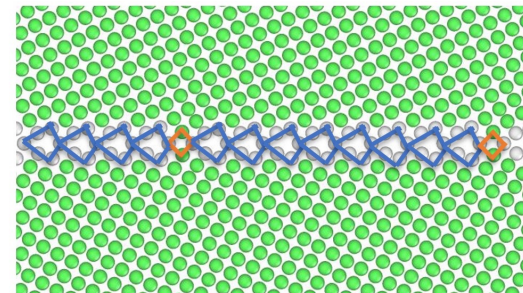
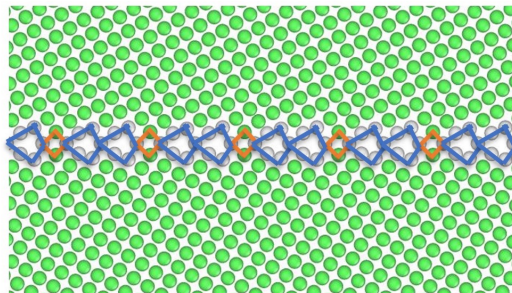
$\Sigma 25(0\ 3\ 4): |2A-B|$



$\Sigma 17(0\ 3\ 5): |A-2B|$



$\Sigma 185(0\ 9\ 17): |A-8B|$



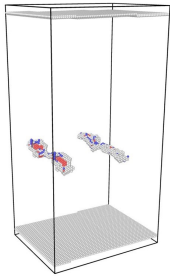
Model system

θ (°)	CSL	γ_{GB} (mJ/m ²)	v_{GB} (10 ⁻³ Å ³ /Å ²)	SU
1.71	$\Sigma 2245(0\ 33\ 34)$	160	22	32A-B
3.27	$\Sigma 613(0\ 17\ 18)$	257	44	16A-B
6.03	$\Sigma 181(0\ 9\ 10)$	383	8	8A-B
10.39	$\Sigma 61(0\ 5\ 6)$	533	68	4A-B
16.26	$\Sigma 25(0\ 3\ 4)$	677	150	2A-B
22.62	$\Sigma 13(0\ 2\ 3)$	790	153	A-B
28.07	$\Sigma 17(0\ 3\ 5)$	909	230	A-2B
31.89	$\Sigma 53(0\ 5\ 9)$	969	247	A-4B
34.21	$\Sigma 185(0\ 9\ 17)$	983	233	A-8B
35.49	$\Sigma 689(0\ 17\ 33)$	1013	145	A-16B
36.17	$\Sigma 2657(0\ 33\ 65)$	978	263	A-32B
36.87	$\Sigma 5\ (0\ 1\ 2)$	953	258	B

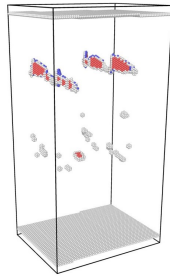
Three Different Modes of Interaction for Grain Boundaries Depending on Structure

Mode 1:
 $\Sigma 2245(0\ 33\ 34)$

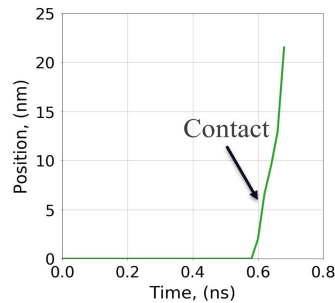
(a1) $t = 0.64\text{ ns}$



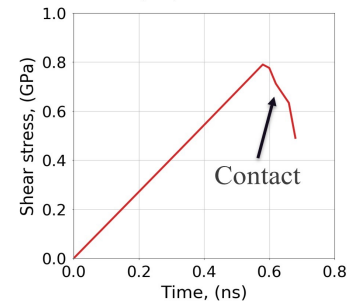
(a2) $t = 0.68\text{ ns}$



(a3) x vs t



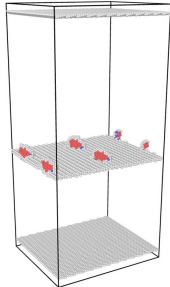
(a4) τ vs t



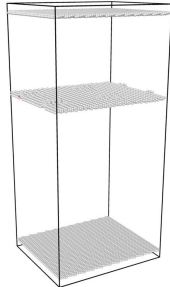
No Change
in Mobility

Mode 2:
 $\Sigma 13(0\ 2\ 3)$

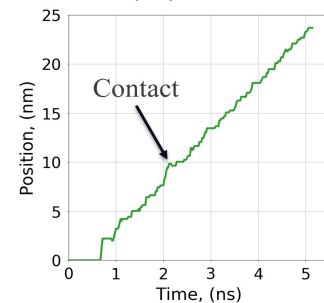
(b1) $t = 2.2\text{ ns}$



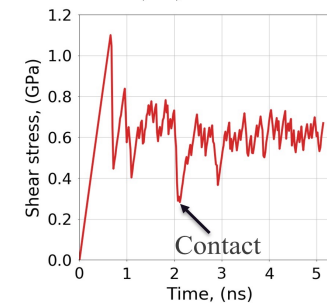
(b2) $t = 4.0\text{ ns}$



(b3) x vs t



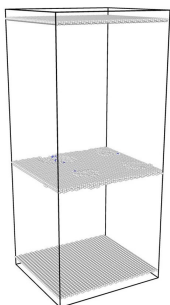
(b4) τ vs t



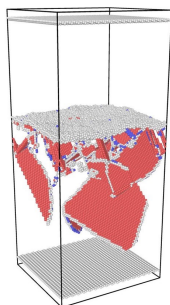
Minor
change in
Mobility

Mode 3:
 $\Sigma 5(0\ 1\ 2)$

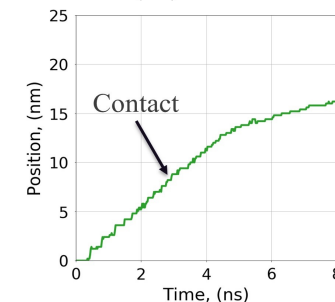
(c1) $t = 3.5\text{ ns}$



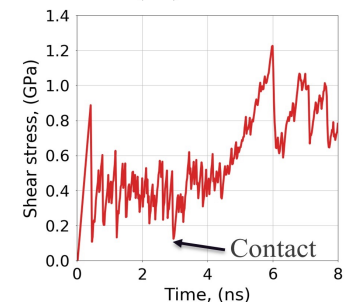
(c2) $t = 8.0\text{ ns}$



(c3) x vs t



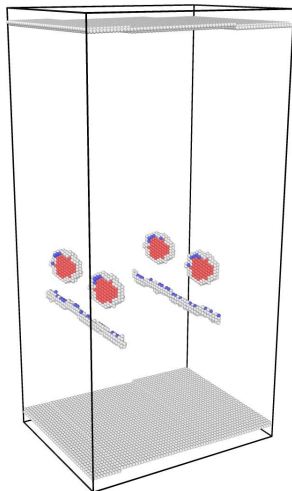
(c4) τ vs t



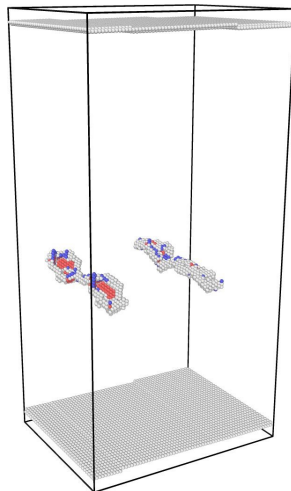
Significant
change in
Mobility

Mode 1: $\Sigma 2245(0\ 33\ 34)$

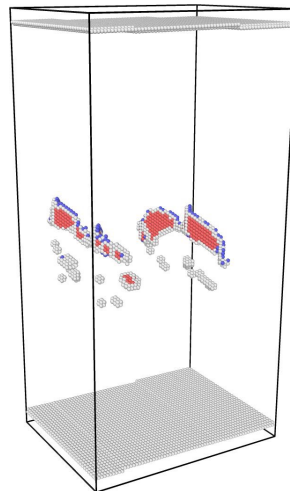
(a) $t = 0.62\text{ ns}$



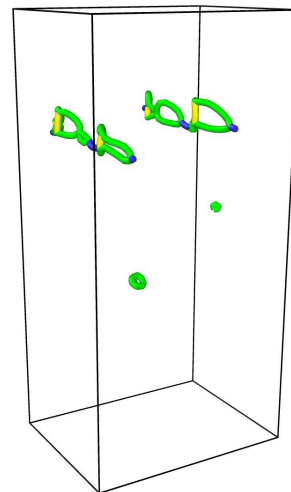
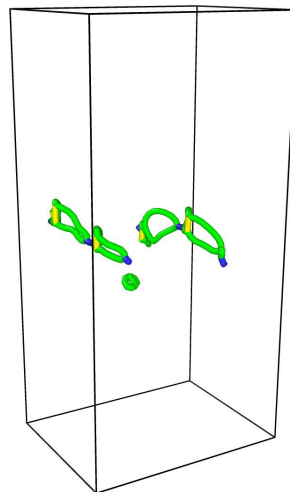
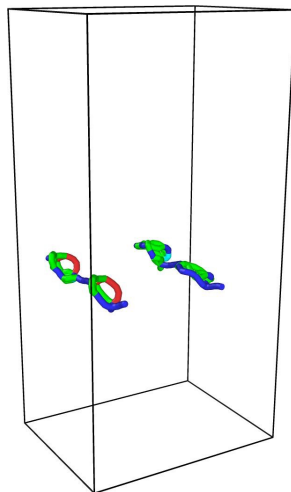
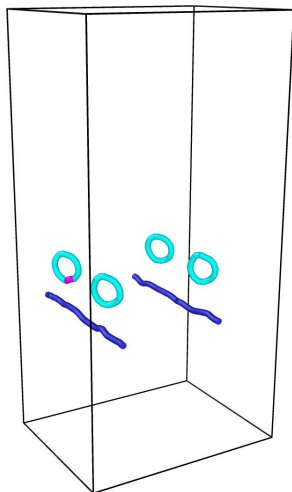
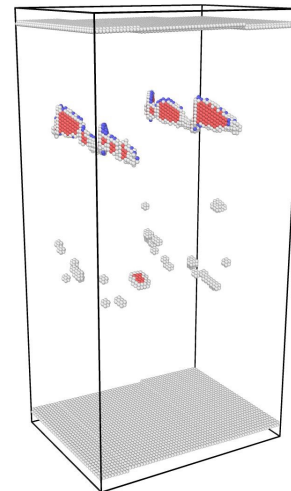
(b) $t = 0.64\text{ ns}$



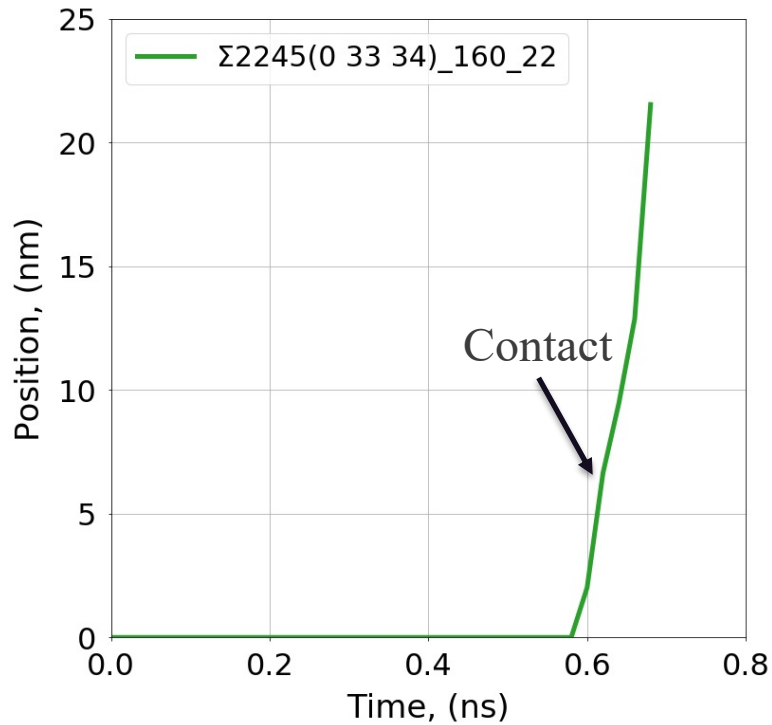
(c) $t = 0.66\text{ ns}$



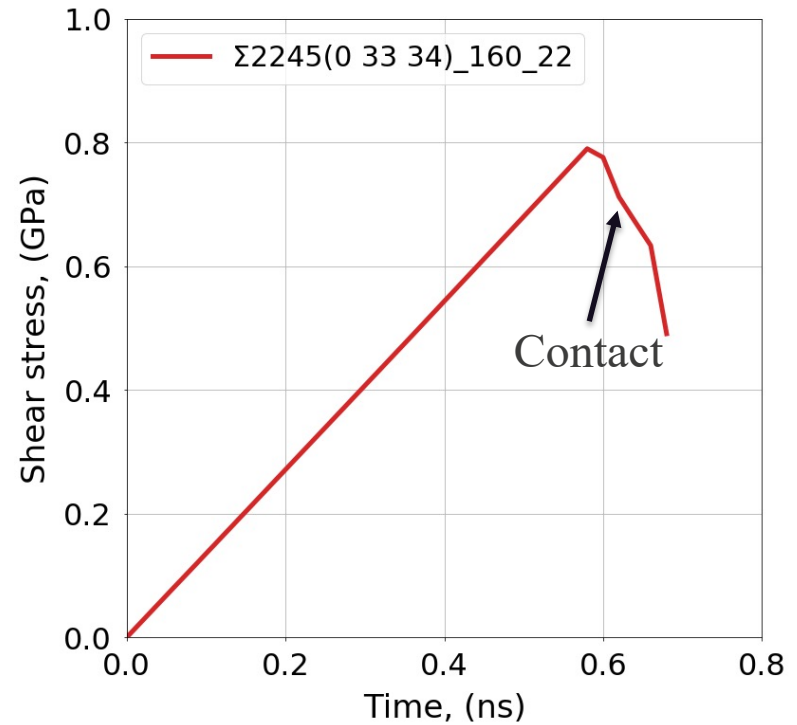
(d) $t = 0.68\text{ ns}$



Mode 1



(a) GB position vs t

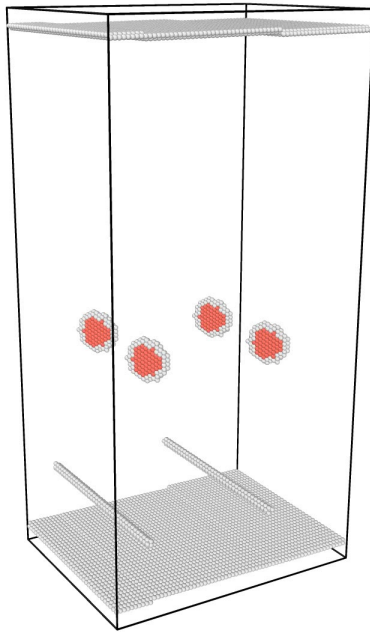


(b) Shear stress vs t

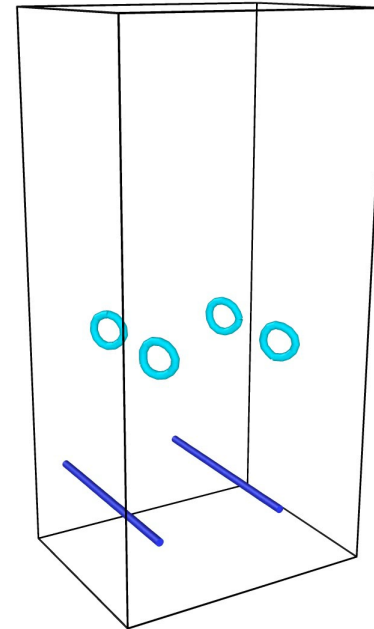
No appreciable slow-down after interaction.

Mode 1: $\Sigma 2245(0\ 33\ 34)$

Defects atoms



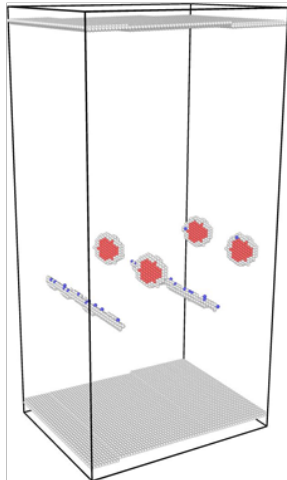
Dislocation lines



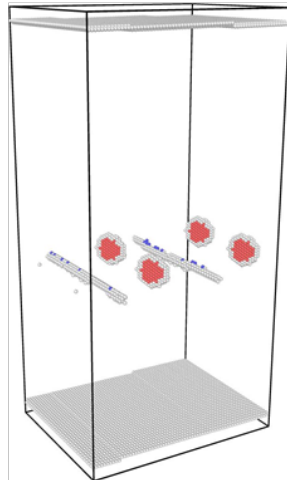
Vacancy (clusters) left behind after interaction.

Behavior Changes in Frank Loops moved w.r.t to Structural unit B (full Dislocation)

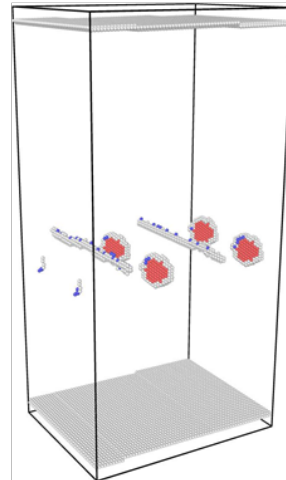
(a) $t = 0.62$ ns



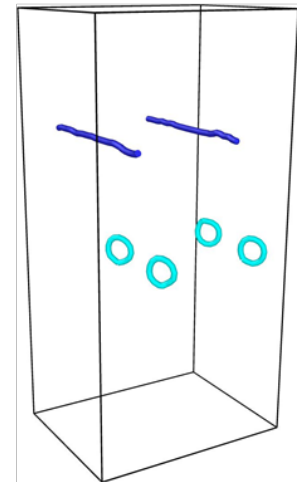
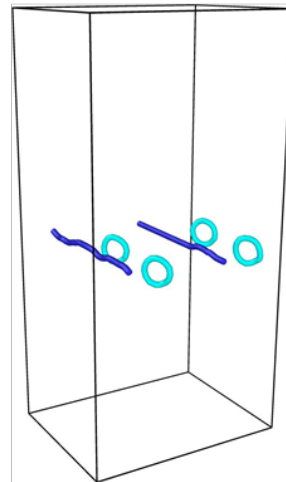
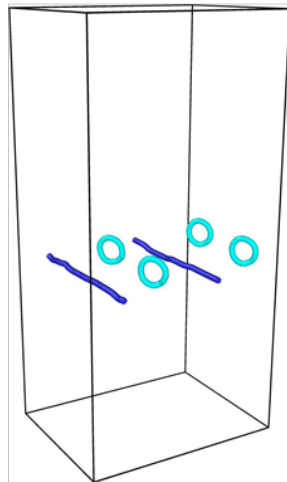
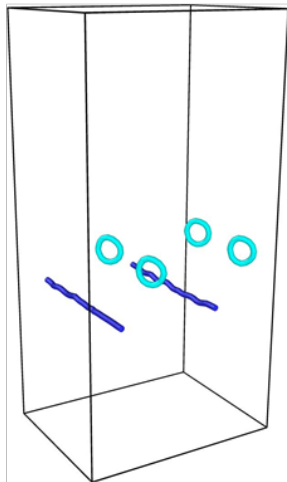
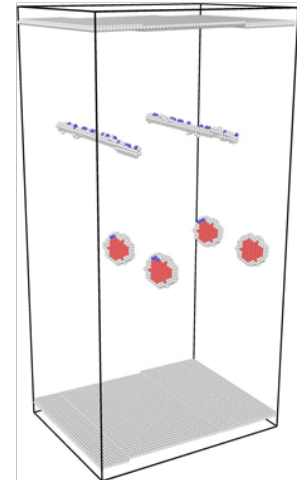
(b) $t = 0.64$ ns



(c) $t = 0.76$ ns

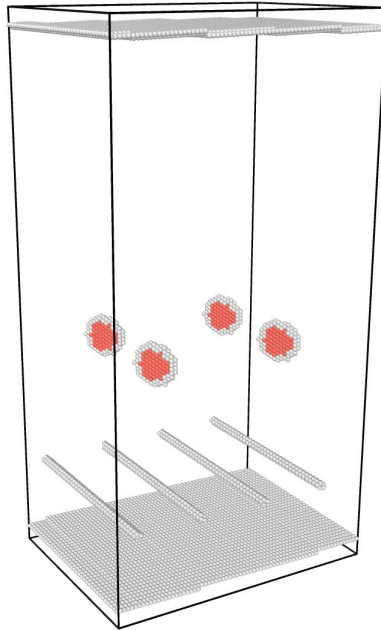


(d) $t = 0.68$ ns

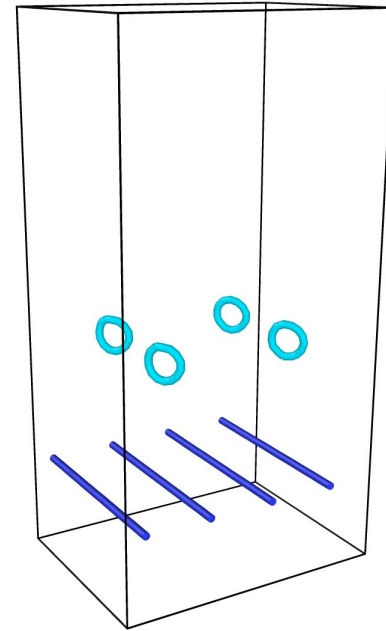


$\Sigma 613(0\ 17\ 18)$

Defects atoms



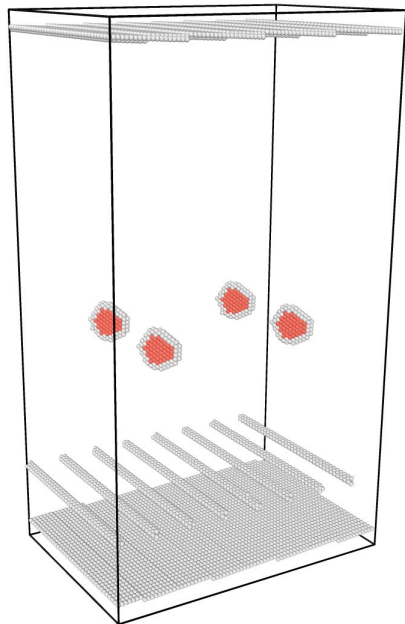
Dislocation lines



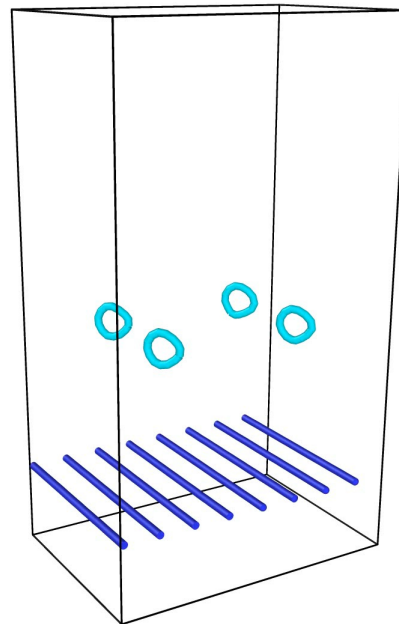
Vacancy (clusters) left behind after interaction.

$\Sigma 181(0\ 9\ 10)$

Defects atoms



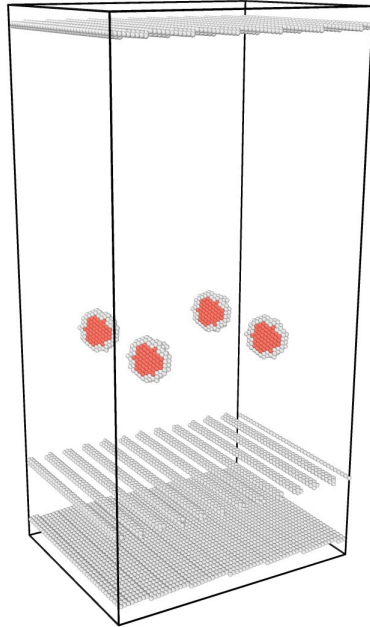
Dislocation lines



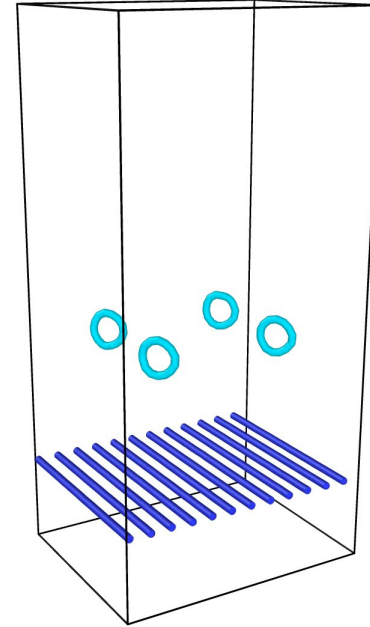
Vacancy (clusters) left behind after interaction.

$\Sigma 61(0\ 5\ 6)$

Defects atoms



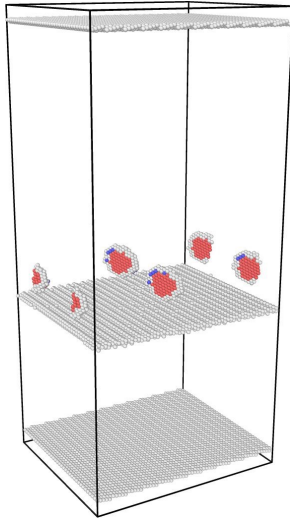
Dislocation lines



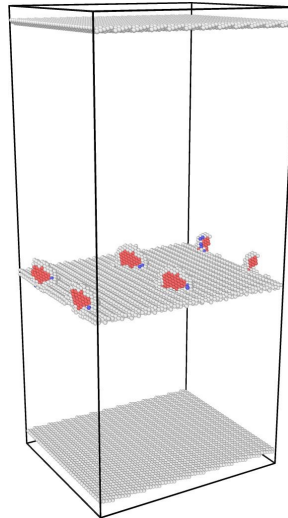
Vacancies left behind after interaction.

Mode 2: $\Sigma 13(0\ 2\ 3)$

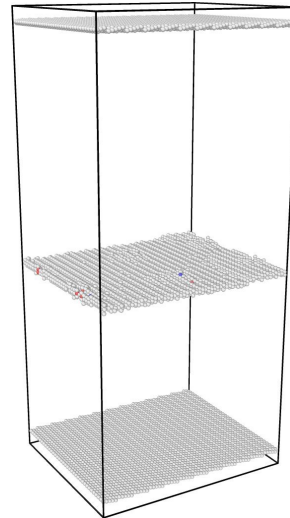
(a) $t = 2.0\text{ ns}$



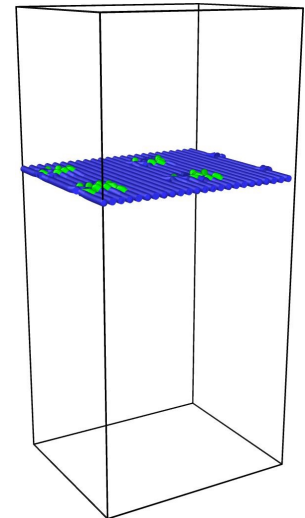
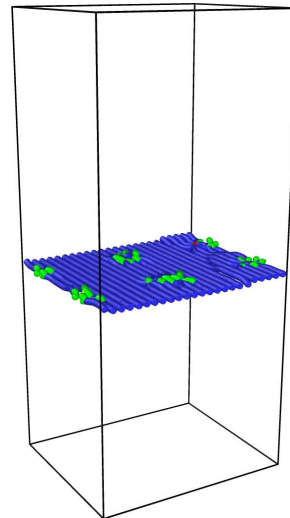
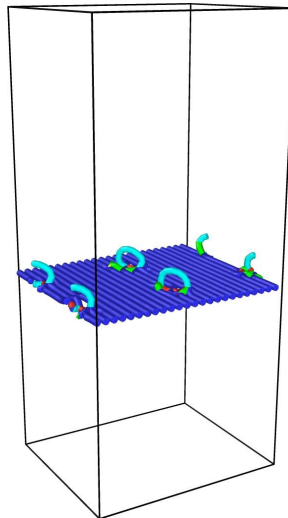
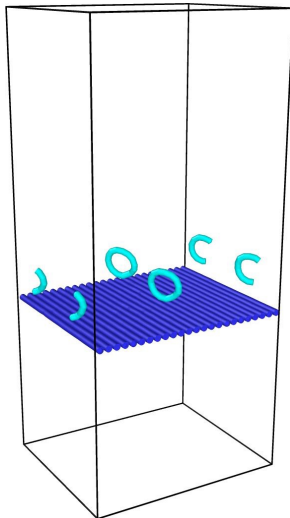
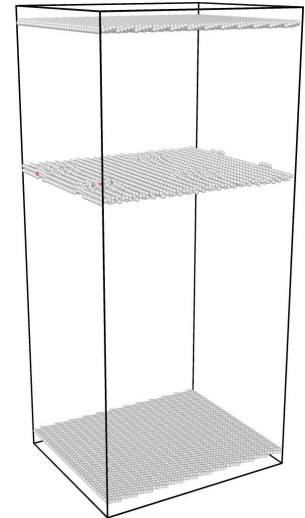
(b) $t = 2.2\text{ ns}$



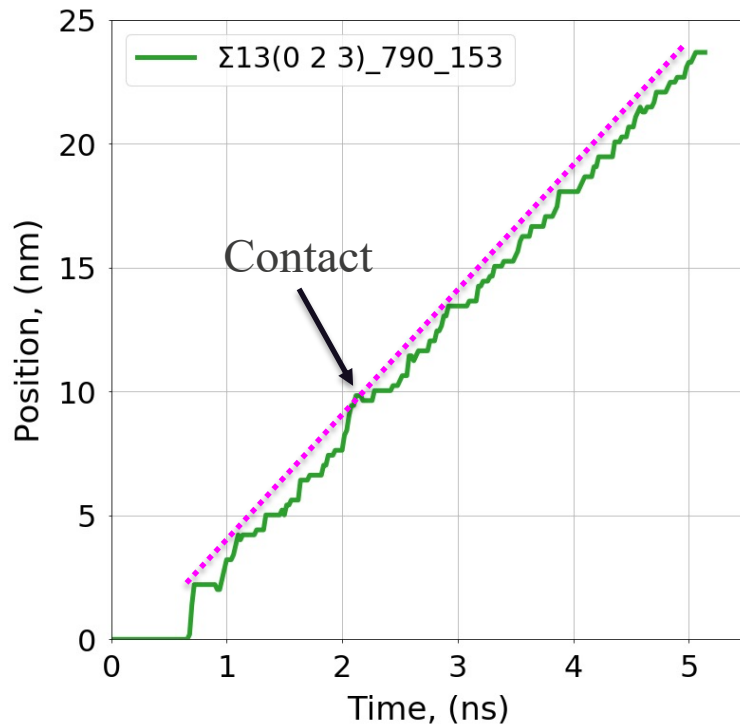
(c) $t = 2.5\text{ ns}$



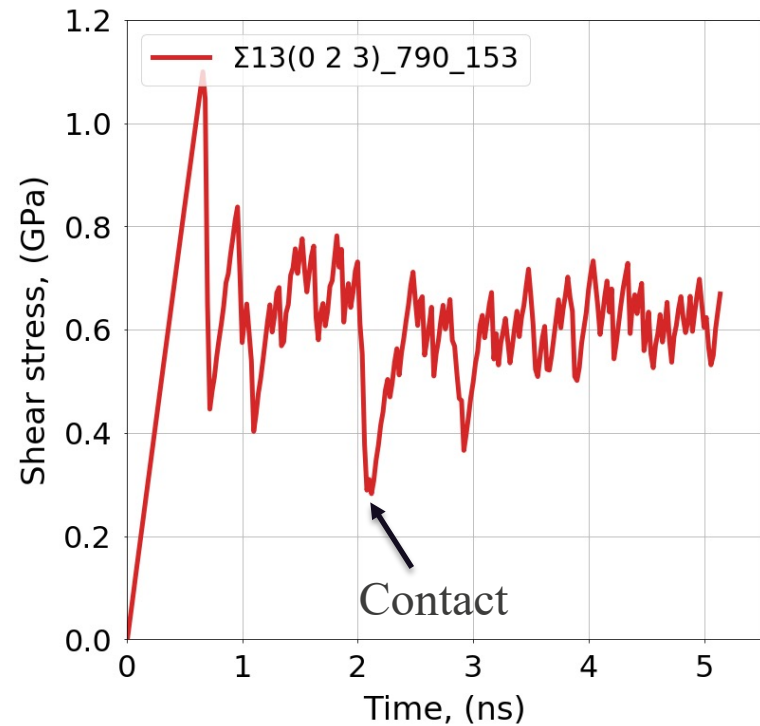
(d) $t = 4.0\text{ ns}$



Mode 2: $\Sigma 13(0\ 2\ 3)$



(a) GB position vs. t

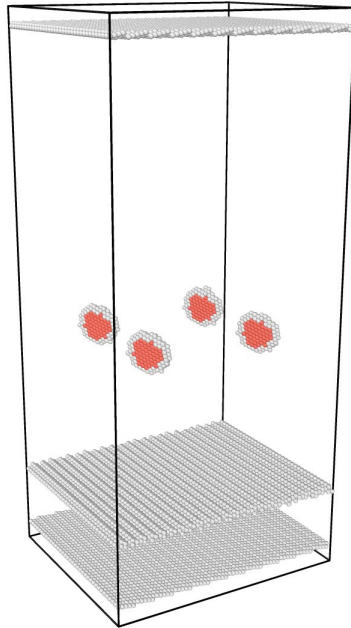


(b) Shear stress vs. t

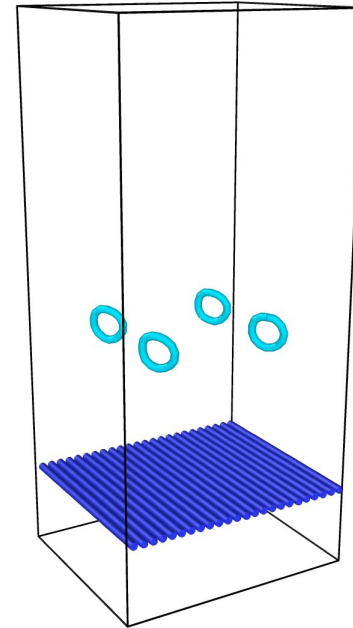
No appreciable slow-down after interaction.

Mode 2: $\Sigma 13(0\ 2\ 3)$

Defects atoms



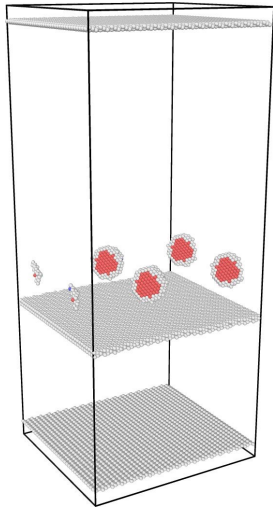
Dislocation lines



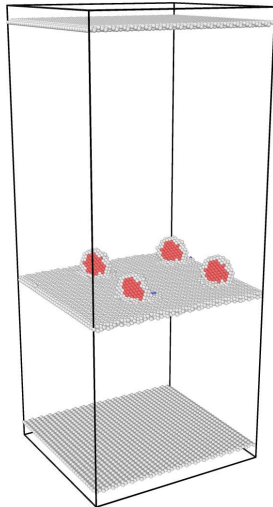
Complete absorption, no vacancy left behind.

Mode 3: $\Sigma 5(0\ 1\ 2)$

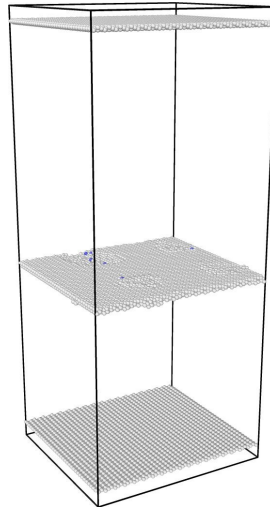
t = 2.5 ns



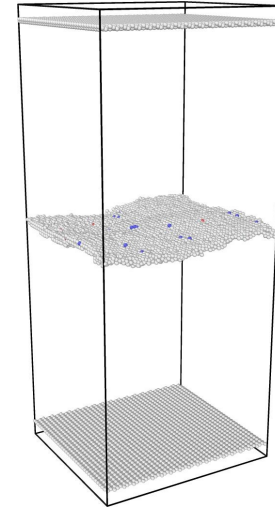
t = 3.0 ns



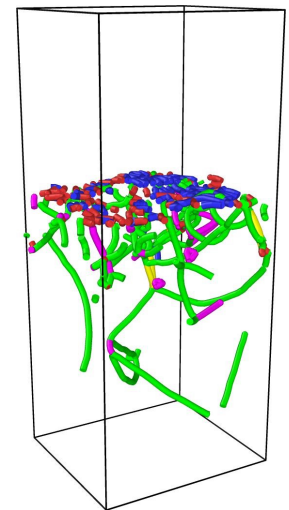
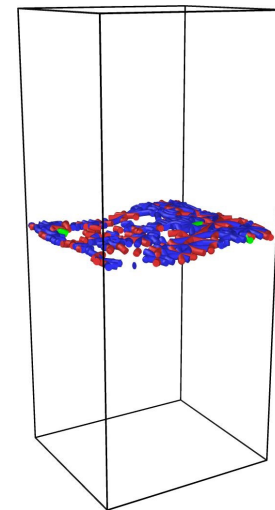
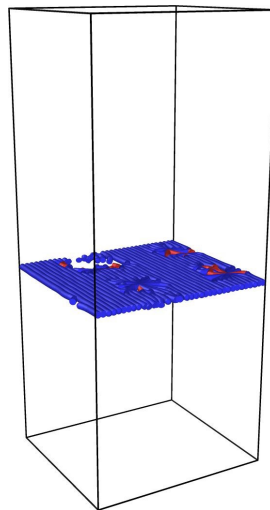
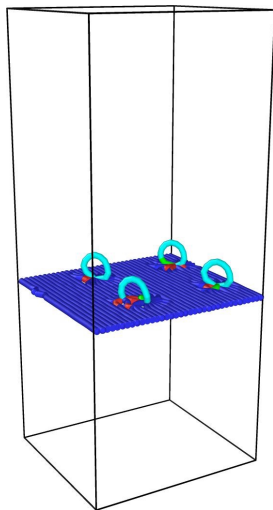
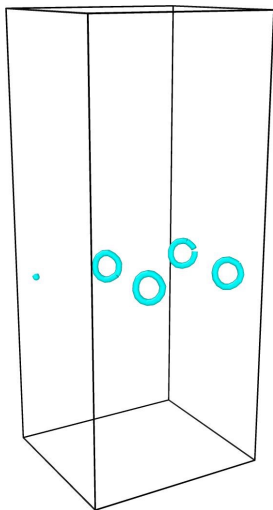
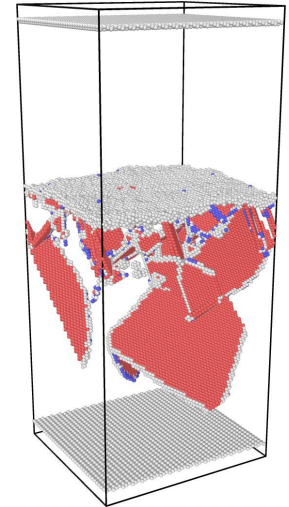
t = 3.5 ns



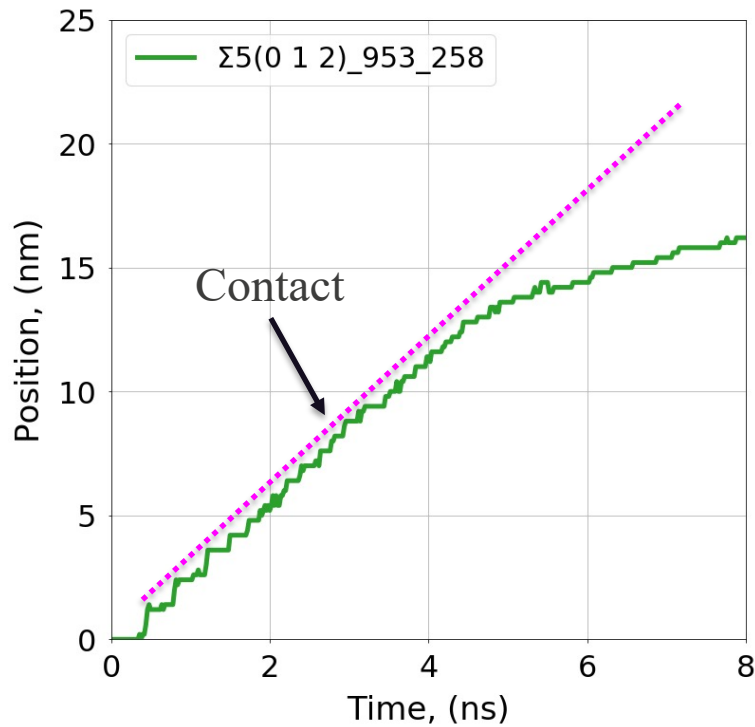
t = 5.0 ns



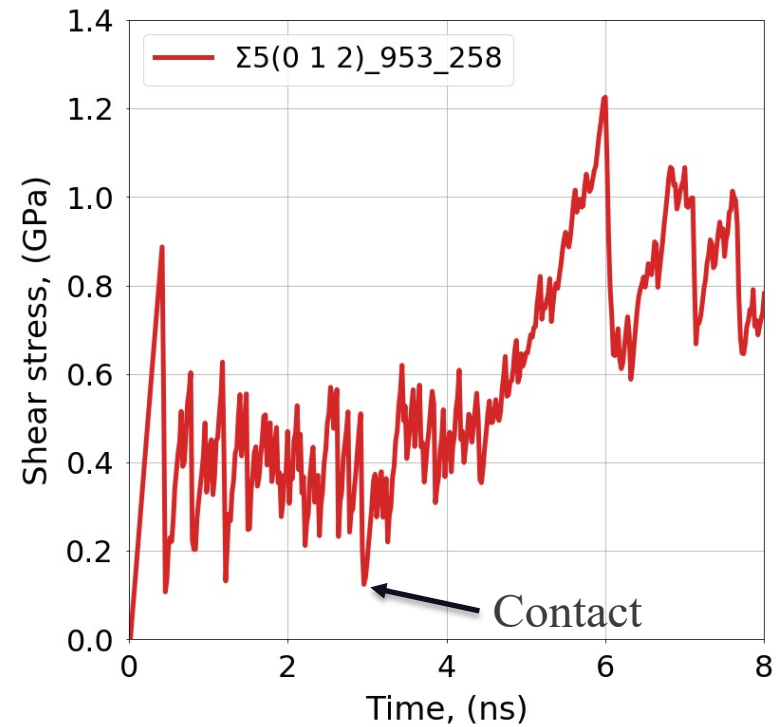
t = 8.0 ns



Mode 3: $\Sigma 5(0\ 1\ 2)$



(a) GB position vs t

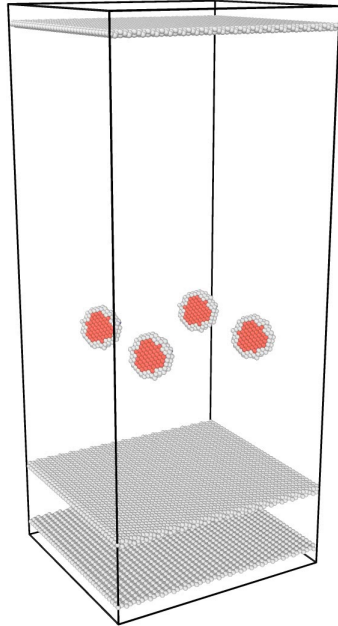


(b) Shear stress vs t

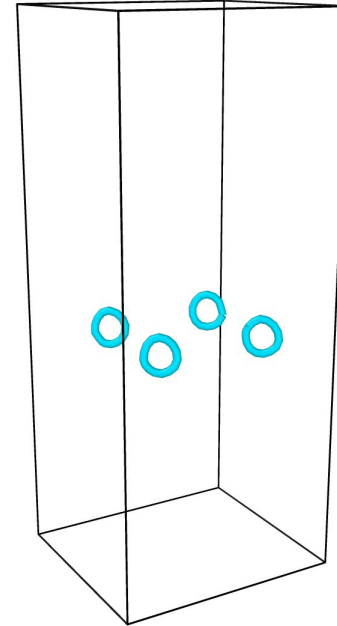
Significant slow-down after interaction.

Mode 3: $\Sigma 5(0\ 1\ 2)$

Defects atoms



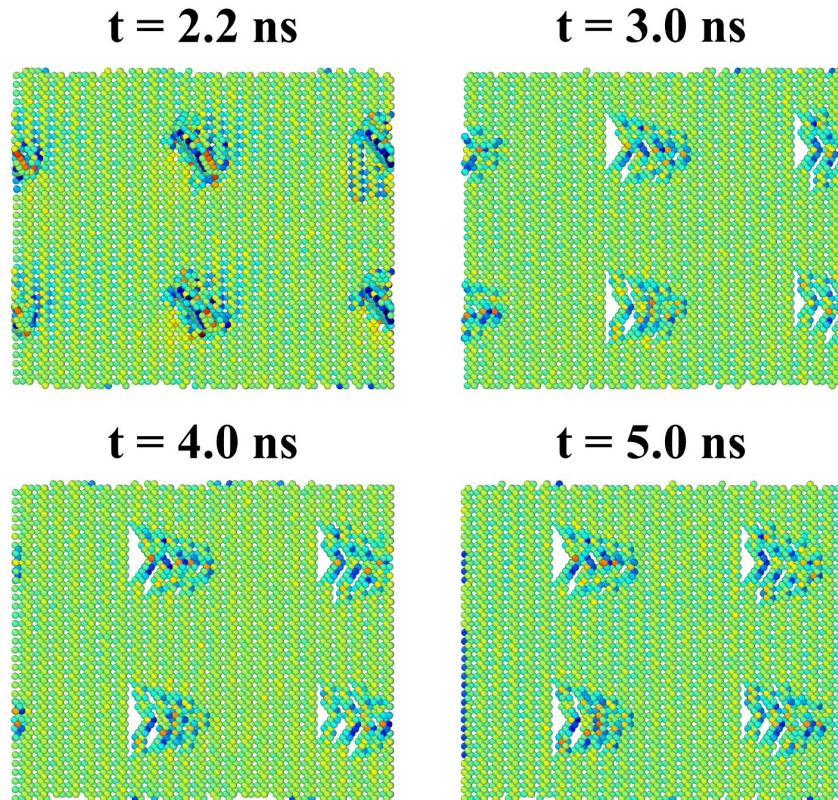
Dislocation lines



GB slows down appreciably after prismatic loop absorption, followed by dislocation emission.

Differences in Regions of Maximum Shear Stress

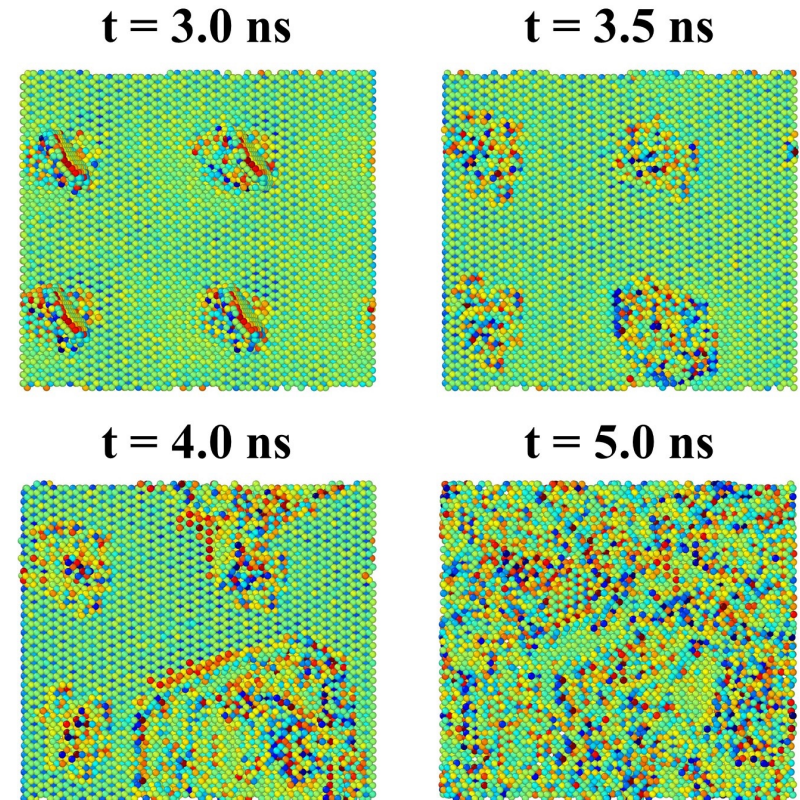
(a) Mode 2: $\Sigma 13(0\ 2\ 3)$



Shear stress (GPa)
-4  6

B SU separated by SU A

(b) Mode 3: $\Sigma 5(0\ 1\ 2)$



Shear stress (GPa)
-5  4

Interconnected SU B

Summary

θ (°)	Structural Unit	Mode of Interaction	GB slowing down?	GB roughening ?
0 ~ 20	$n1A+n2B$ $n1/n2 > 1$	Partial absorption, leaving behind vacancy (clusters).	No	No
20 ~ 32	$n1A+n2B$ $0.25 \leq n1/n2 \leq 1$	Complete absorption.	No	No
32 ~ 40	$n1A+n2B$ $n1/n2 < 0.25$	Complete absorption, leaving behind vacancies, followed by dislocation emission.	Yes	Yes
> 40	$n2B+n3C$	Complete absorption, leaving behind vacancies.	Yes	Yes

- Each B structural unit provides one perfect dislocation line that can interact with Frank loop and accommodate the interstitial atoms (recall we introduce interstitial type Frank loops here, which is nothing but a circular disk of interstitial atoms).
- With increasing misorientation angle (0° - 40°), there is an increase in density of B structural unit, and therefore enhanced ability of the GB to absorb the Frank loop.

The Transition Between the Modes Changes with Frank Loop Size and GB structure

θ (°)	CSL	Flat	Zig-zag	Flat ($D_{\text{loop}} = 4 \text{ nm}$)
1.71	$\Sigma 2245(0\ 33\ 34)$	Mode 1	N/A	N/A
3.27	$\Sigma 613(0\ 17\ 18)$	Mode 1	N/A	N/A
6.03	$\Sigma 181(0\ 9\ 10)$	Mode 1	N/A	N/A
10.39	$\Sigma 61(0\ 5\ 6)$	Mode 1	N/A	N/A
16.26	$\Sigma 25(0\ 3\ 4)$	Mode 1	N/A	Mode 1
22.62	$\Sigma 13(0\ 2\ 3)$	Mode 2	N/A	Mode 1
28.07	$\Sigma 17(0\ 3\ 5)$	Mode 2	Mode 2	Mode 1
31.89	$\Sigma 53(0\ 5\ 9)$	Mode 2	Quasi-Mode 2*	Mode 1
34.21	$\Sigma 185(0\ 9\ 17)$	Mode 3	Mode 2	Mode 1
35.49	$\Sigma 689(0\ 17\ 33)$	Mode 3	Mode 2	Mode 3
36.17	$\Sigma 2657(0\ 33\ 65)$	Mode 3	Mode 3	Mode 3
36.87	$\Sigma 5(0\ 1\ 2)$	Mode 3	N/A	Mode 3